

A Lanczos algorithm for linear response

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Abstract

An iterative algorithm is presented for solving the RPA equations of linear response. The method optimally computes the energy-weighted moments of the strength function, allowing one to match the computational effort to the intrinsic accuracy of the basic mean-field approximation, avoiding the problem of solving very large matrices. For local interactions, the computational effort for the method scales with the number of particles N_p as $O(N_p^3)$.

I. INTRODUCTION

In a number of branches of physics, mean field theory gives a remarkably effective approximation to the ground state. Similarly, for the response of the system to small perturbations, time-dependent mean field theory is a useful extension. This is the experience in nuclear physics [1,2], atomic and molecular physics [3–8] and condensed matter physics [9,10]. There are of course intrinsic limitations to these approximations, but equally pressing is the large computational resources required for calculations of systems of interest. This is our motiva-

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tion to look for algorithms that better match the computational effort to the intrinsic limits of the approximation.

We take our inspiration from the Lanczos algorithm [11], which is best known in many-body physics for extracting low-lying eigenstates of very large Hamiltonian matrices [12,13]. When dealing with large spaces, the computational question often comes down to the number of times the Hamiltonian operates on a state vector. Depending on the Hamiltonian and the starting vector, the Lanczos algorithm is able to extract an accurate ground state vector in a basis of 10^{5-6} states with a few hundred Hamiltonian operations. The algorithm may be viewed as a numerically stable technique [14] to compute moments of the Hamiltonian with respect to some initial state Ψ_0 , that is, $\mu_k \equiv \langle \Psi_0 | \hat{H}^k | \Psi_0 \rangle$. For large k , μ_k is dominated by the extremal eigenvalues [15], which are thus available for recovery.

The Lanczos algorithm has also been applied to many other topics in atomic, molecular, solid state, and nuclear physics, including computation of the S-matrix [16], time-evolution of wave packets [17], level densities [18], and the continued-fraction expansion of the resolvent or Green's function [19]. Particularly relevant to us is the application to strength functions. The strength function S for an operator \hat{Q} on a state i is defined

$$S(E) \equiv \sum_f \delta(E - E_f + E_i) \left| \langle f | \hat{Q} | i \rangle \right|^2. \quad (1)$$

A powerful technique to calculate the strength function, successfully applied to the nuclear shell model [13,20], uses the Lanczos algorithm with a starting vector $|\Psi_0\rangle = \hat{Q} |i\rangle / \langle i | \hat{Q}^2 | i \rangle^{1/2}$. The Lanczos algorithm implicitly computes the moments

$$M_k = \int dE (E - E_i)^k S(E)$$

of the strength function. After a few tens of iterations one can accurately reconstruct the distribution of the exact strength function.

In many cases, however, the matrix elements of the operator \hat{Q} are sensitive to correlations in the ground state, and then the size of the wave function basis in the straightforward Hamiltonian approach becomes problematic. In this situation, the time-dependent mean-field theory offers a reasonable compromise. The small amplitude theory, the RPA or linear

response, can be cast into a matrix form in a particle-hole basis. However, the RPA matrix is not symmetric as required by the Lanczos algorithm. The matrix equation is commonly written as

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix} \begin{pmatrix} \vec{x} \\ \vec{y} \end{pmatrix} = \omega \begin{pmatrix} \vec{x} \\ \vec{y} \end{pmatrix} \quad (2)$$

where \mathbf{A} and \mathbf{B} are particle-hole Hamiltonian matrices, ω is the eigenfrequency, and \vec{x} and \vec{y} are the vectors of positive- and negative-frequency particle-hole amplitudes, respectively. An important property of the RPA equation is that eigenvectors come in conjugate pairs: in equation (2) (\vec{y}, \vec{x}) is also an eigenvector with eigenfrequency $-\omega$. For the linear response, the matrix element between the RPA ground state $|0\rangle$ and an excited state $|\omega\rangle$ may be expressed as

$$\langle \omega | \hat{Q} | 0 \rangle = (\vec{q}, \vec{q}) \cdot \begin{pmatrix} \vec{x} \\ \vec{y} \end{pmatrix} \quad (3)$$

where \vec{q} is the vector of particle-hole matrix elements and the vector (\vec{x}, \vec{y}) is normalized as $1 = \vec{x} \cdot \vec{x} - \vec{y} \cdot \vec{y}$.

There are a number of ways to introduce a Lanczos-type algorithm for the RPA matrix. The method we describe here has the advantages that it preserves the form eq.(2) of the RPA matrix and it produces strength functions that respect sum rules. We seek a new basis of vectors $|Z_i\rangle := (\vec{X}_i, \vec{Y}_i)$ where the matrices of column vectors $\mathbf{U} := (\vec{X}_1, \vec{X}_2, \vec{X}_3, \dots)$ and $\mathbf{V} := (\vec{Y}_1, \vec{Y}_2, \vec{Y}_3, \dots)$ transform the RPA matrix as

$$\begin{pmatrix} \mathbf{U}^T & -\mathbf{V}^T \\ -\mathbf{V}^T & \mathbf{U}^T \end{pmatrix} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix} \begin{pmatrix} \mathbf{U} & \mathbf{V} \\ \mathbf{V} & \mathbf{U} \end{pmatrix} = \begin{pmatrix} \mathbf{A}' & \mathbf{B}' \\ -\mathbf{B}' & -\mathbf{A}' \end{pmatrix} \quad (4)$$

where the transformed matrices \mathbf{A}' and \mathbf{B}' are now tridiagonal:

$$\mathbf{A}' = \begin{pmatrix} e_1 & a_1 & 0 & & \\ a_1 & e_2 & a_2 & & \\ 0 & a_2 & e_3 & & \\ & & & \ddots & \end{pmatrix}, \mathbf{B}' = \begin{pmatrix} d_1 & b_1 & 0 & & \\ b_1 & d_2 & b_2 & & \\ 0 & b_2 & d_3 & & \\ & & & \ddots & \end{pmatrix} \quad (5)$$

The Lanczos basis vectors and matrix elements are generated iteratively as follows. Suppose we have the vectors $|Z_1\rangle, \dots, |Z_n\rangle$ already computed, together with the transformed

matrix up to $e_{n-1}, d_{n-1}, a_{n-1}$ and b_{n-1} . The iteration starts by applying the RPA matrix in eqn. (2) to the vector $|Z_n\rangle$,

$$|Z_t\rangle = \begin{pmatrix} \vec{X}_t \\ \vec{Y}_t \end{pmatrix} = \begin{pmatrix} \mathbf{A}\vec{X}_n + \mathbf{B}\vec{Y}_n \\ -\mathbf{B}\vec{X}_n - \mathbf{A}\vec{Y}_n \end{pmatrix} \quad (6)$$

The diagonal elements e_n and d_n are now easily computed:

$$\begin{aligned} e_n &= \vec{X}_t \cdot \vec{X}_n - \vec{Y}_t \cdot \vec{Y}_n \\ d_n &= \vec{X}_t \cdot \vec{Y}_n - \vec{Y}_t \cdot \vec{X}_n. \end{aligned} \quad (7)$$

We next project out $|Z'_t\rangle$, the component of $|Z_t\rangle$ that is orthogonal to the space $|Z_1\rangle, \dots, |Z_n\rangle$. This can be done conveniently by using the matrix elements in (5) that have already been calculated,

$$|Z'_t\rangle = \begin{pmatrix} \vec{X}'_t \\ \vec{Y}'_t \end{pmatrix} = \begin{pmatrix} \vec{X}_t - e_n \vec{X}_n + d_n \vec{Y}_n - a_{n-1} \vec{X}_{n-1} + b_{n-1} \vec{Y}_{n-1} \\ \vec{Y}_t - d_n \vec{X}_n + e_n \vec{Y}_n - b_{n-1} \vec{X}_{n-1} + a_{n-1} \vec{Y}_{n-1} \end{pmatrix} \quad (8)$$

The norm of the vector $|Z'_t\rangle$ is then computed as

$$\mathcal{N} = \vec{X}'_t \cdot \vec{X}'_t - \vec{Y}'_t \cdot \vec{Y}'_t \quad (9)$$

The norm can be negative, and the definition of the new vector $|Z_{n+1}\rangle$ depends on the sign. In fact, because we are actually doing *block*-Lanczos, implicitly operating not only on the vector (X, Y) but also its RPA conjugate (Y, X) simultaneously, there is a degree of freedom, corresponding to a hyperbolic rotation, in choosing the new vector. The simplest choice for the vectors and corresponding RPA matrix elements is

$$|Z_{n+1}\rangle = \frac{1}{\sqrt{\mathcal{N}}} \begin{pmatrix} \vec{X}'_t \\ \vec{Y}'_t \end{pmatrix}, \quad a_{n+1} = \sqrt{\mathcal{N}}, \quad b_{n+1} = 0; \quad \mathcal{N} > 0 \quad (10)$$

and

$$|Z_{n+1}\rangle = \frac{1}{\sqrt{-\mathcal{N}}} \begin{pmatrix} \vec{Y}'_t \\ \vec{X}'_t \end{pmatrix}, \quad a_{n+1} = 0, \quad b_{n+1} = \sqrt{-\mathcal{N}}, \quad \mathcal{N} < 0 \quad (11)$$

This completes the iteration cycle.

In analogy with the application to strength functions in the nuclear shell model, we start with the vector given by

$$|Z_1\rangle = \begin{pmatrix} \vec{X}_1 \\ \vec{Y}_1 \end{pmatrix} = \begin{pmatrix} \vec{q} \\ 0 \end{pmatrix}; \quad (12)$$

With such a starting vector the algorithm manifestly preserves the energy-weighted sum rules:

$$M_k = \sum_{\nu} \omega_{\nu}^k \langle \omega_{\nu} | \hat{Q} | 0 \rangle^2, \quad k \text{ odd}. \quad (13)$$

Using the eigenvector representation of the RPA matrix, one can show

$$M_k = \frac{1}{2}(\vec{q}, \vec{q}) \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix}^k \begin{pmatrix} \vec{q} \\ -\vec{q} \end{pmatrix}, \quad k \text{ odd}. \quad (14)$$

With our method the n -th iterate respects the odd- k sum rules for $k \leq 2n - 1$.

We now illustrate the method with a very simple model, a collective particle-hole interaction fragmented by single-particle energies. We consider states $i = 1, \dots, N$ with matrix elements $A_{ij} = \epsilon_i \delta_{ij} + \kappa q_i q_j$ and $B_{ij} = \kappa q_i q_j$. Here ϵ represents the energy spacing of the particle-hole configurations, κ is the strength of the collective coupling to the field Q , and the components of the vector $q_i \propto i(N - i) \times r$, where the r are Gaussian distributed random amplitudes, and normalize $|q|^2 = 1$. The factor $i(N - i)$ weights the collective response towards the middle of the excitation spectrum. The parameter κ should be positive for a repulsive collective interaction such as the Coulomb that generates plasmons.

In Fig. 1 we show the strength function for such an RPA matrix in a space of 500 states, with parameter values given in the caption. The parameters were chosen to obtain moderate collectivity, with a strong but broadly-fragmented collective excitation distributed over the spectrum. Fig. 1 also displays the $n=3, 10$, and 50 approximants to the strength function, where n is the number of Lanczos vectors $|Z_i\rangle$, or, equivalently, the number of multiplications with the RPA matrix. One sees that with a handful of states, one state closely approximates the collective excitation and the others distribute themselves over the remaining spectrum. A better way to see the convergence of the strength function is to plot its integral, $I(\omega) = \sum_{\nu} \Theta(\omega - \omega_{\nu}) \langle \omega_{\nu} | Q | 0 \rangle^2$. This is shown in Fig. 2 for $n=3$ and 10. After 50 iterations the integral of the strength function is virtually indistinguishable from the exact solution.

We mention that the algorithm does not explicitly preserve the total strength M_0 . If there were no correlations in the ground state, that is, if the vectors Y_i all vanished, then the total strength would be $|q|^2 = 1$. The non-trivial deviations from 1 in our examples are related to the amount of correlations in the ground state. This is illustrated in Fig. 3, which is the integrated strength function for a model identical to that in Figs. 1,2 except that the collective interaction is attractive rather than repulsive. Here the total strength is about 3.7, i.e. quite different from 1. Fig. 3 illustrates how with $n = 3$ and 10 the total approximate strength converges rapidly to the exact value. (In the repulsive model of Fig. 2 the total strength had already converged by $n = 3$.) Although we cannot prove this rapid convergence in all cases, it seems likely in light of the strong constraints imposed by the odd- k sum rules.

We anticipate that the algorithm will be particularly useful in problems which require a single-particle dimensionality of the order of tens or hundreds of thousands, but which allow a sparse matrix approximation for the Hamiltonian, such as the local density approximation. This applies to molecular and condensed matter physics modeled with the Kohn-Sham equations, and to nuclear physics for excitations in deformed nuclei [2]. With the LDA Hamiltonian, an efficient particle-hole representation can be constructed from the orbital representation of holes and the coordinate-space representation of particles [21]. The computational difficulty for the basic matrix-vector multiplication then scales as the number of particles N_p and the dimensionality of the single-particle space M as $MN_p^2 \sim N_p^3$. Only a fixed number of these operations, of the order of ten, are needed to obtain the strength function to the accuracy of the fundamental mean field approximation. Thus the overall scaling of the method is $O(N_p^3)$.

This study arose in the program at the Institute for Nuclear Theory, “Numerical methods for strongly interacting quantum systems”, and we wish to thank J. Carlson and R. Wiringa for providing that forum. G.B. also thanks K. Yabana for many discussions. Financial support was provided by the INT under Department of Energy Grant FG06-90ER40561 and by Department of Energy Grant DE-FG02-96ER40985.

FIGURES

FIG. 1. Strength function for the model described in the text with $\kappa = 10$ and $\epsilon = 0.1$ (in arbitrary units) for 500 states, and the Lanczos approximants for 5, 10, and 50 Lanczos vectors. The scales for the abscissae are different because the strength is fragmented over a different number of states.

FIG. 2. Integrated strength function for the model described in Fig. 1. For 50 Lanczos vectors the integrated strength is virtually indistinguishable on this graph from the full calculation.

FIG. 3. The same as figure 2, except with the collective interaction is attractive, $\kappa = -10$. Notice that the total strength is not constrained, as described in the text, but has converged by the 10th iteration.

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